

## Conference Paper

# Lattice Boltzmann Simulation of Convection Melting in Complex Heat Storage Systems Filled with Phase Change Materials

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## Abstract

A double-population lattice Boltzmann method is applied to simulate the convection-diffusion phenomena associated with solid-liquid phase transition processes. The research focus is the lattice Boltzmann method advanced to complex multitube heat storage system with different numbers and arrangements of tubes. A systematic comparison of different lattice Boltzmann models for thermal and flow field in the phase-change process is numerically conducted in a square cavity; the numerical results are validated by the literature data. The computational results show how the transient phase-change process, expressed in terms of the volume melt fraction of phase change materials, depends on the thermal and geometrical parameters of the system.

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## 1. Introduction

The fundamentals of heat transfer and flow in phase change materials (PCM) have received considerable attention during the past two decades due to its potential for thermal energy storage systems. There exists a wide range of applications for such systems [1–3], such as energy storage in buildings, electronics cooling, material processing, and thermal management of spacecraft. Theoretical, numerical, and experimental studies in the field have yielded extensive literature on various aspects of the phase-change problems, including basic studies of phase-change phenomena [4], material properties [5], experimental methods, heat transfer enhancement [6–8], mathematical modeling, and numerical techniques [9–11]. Among them, numerical simulation is under a major focus, because efficient and powerful computation can significantly improve the understanding of the convection melting processes in heat

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storage system. It is concluded in the critical review of Agyenim et al. [7] that the most common numerical approach used the enthalpy formulation.

Some well-developed methods have been applied to simulate the convection melting models, such as finite difference method (FDM) [12], finite volume method (FVM) [13, 14], finite element method (FEM) [15], and lattice Boltzmann method (LBM) [16]. These numerical simulations are mainly based on two types of grid systems, namely, fixed grid [17] and adaptive grid (or front tracking) [18], in which the enthalpy-based LBM is a newly introduced fixed grid based approach for phase change problems.

The existing mathematical models of the phase change problem are mostly based on continuum approaches. LBM is a relatively new approach that uses simple kinetic models to simulate complicated macroscopic transport phenomena. Owing to its mesoscopic nature, in comparison with conventional fluid dynamics solvers, it offers such advantages as simple calculation procedure, simple and efficient implementation of parallel computation, and easy and robust handling of complex geometries. In 1998, Chen and Doolen [19] first applied LBM to the fluid flow problems. Then, it was developed to solve a wide range of heat transfer problems [20]. Recently, phase change problems have also been investigated by LBM [21]. Since LBM is inherently transient, it is an excellent approach for the investigation of transient phase change process. Specifically, LBM solves the problems by evolution, which agrees well with the real physical melting process. In recent years, the application of LBM to phase change problems has been extensively investigated by many researchers [22–31].

It seems that Miller et al. [22] first developed a simple reaction model for the liquid-solid phase transition in the context of LBM with enhanced collisions. In his work, a two-dimensional test problem of Ga melting and a two-dimensional anisotropic growth of dendrites were presented. Jiaung et al. [23] proposed an extended lattice Boltzmann equation for the simulation of the phase-change problem governed by the heat conduction equation incorporated with enthalpy formation. Chakraborty and Chatterjee, in their outstanding works [16, 21, 24, 25], applied LBM for numerical simulation of conduction-dominated and convection-dominated phase change process (melting and solidification). Huber et al. [26] investigated the coupled thermal convection and pure-substance melting using LBM. The transition from conduction-dominated heat transfer to fully-developed convection was analyzed. Gao et al. [27] performed a lattice Boltzmann simulation of natural convection dominated melting in a rectangular cavity filled with porous media. Eshraghi et al. [28] developed an implicit LBM for heat conduction with phase change, in which the latent heat source term was treated implicitly in the energy equation. Huang and Gong et al. [29, 30] introduced an

enthalpy based LBM for phase change problems. In their works, the phase interface was traced by updating the total enthalpy, and the moving interface was treated by the immersed moving boundary scheme. Fuentes et al. [31] presented a new LBM-MRT hybrid model to simulate melting with natural convection in PCM. In the work, energy equation was solved by a finite difference method, whereas the fluid flow was solved by the multiple relaxation time (MRT) LBM.

As mentioned earlier, phase change problems were numerically investigated by different models in a generalized lattice Boltzmann framework, but no detailed comparison between these models was provided in any reference works. Besides, most of lattice Boltzmann simulations for the phase change problems have been done in a simple cavity, and few study concerned more complex geometries. Therefore, the purpose of the present investigation is threefold: (i) to evaluate the capability of different LBMs for phase change process, that is, the numerical stability of lattice Bhatnagar-Gross-Krook (LBGK) and MRT models for flow field, and the enthalpy-based LBM with basic evolution variable of temperature (TLBM) and enthalpy (HLBM) for thermal field; (ii) to test the heat storage performance for three configurations consisting of a shell with different numbers (one, four, and nine) of heat transfer tubes and different tubes arrangements (inline, staggered, and a novel centrosymmetric design); (iii) to analyze the influence of the Rayleigh and Stefan numbers on the melting dynamics of shell and tube models with various arrangements.

## 2. Methods

### 2.1. Continuum conservation equations

The fundamental equations for thermo-fluidic transport in the presence of melting/solidification (assuming a Newtonian, laminar, and incompressible flow), can be described as follows [16]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \rho \mathbf{f} \quad (2)$$

$$\frac{\partial (\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p \mathbf{u} T) = \nabla \cdot (k \nabla T) + q \quad (3)$$

In the aforementioned equations,  $\rho$ ,  $\mathbf{u}$ ,  $T$ ,  $p$ ,  $\mu$ ,  $C_p$ , and  $k$  are the density, velocity, temperature, pressure, dynamic viscosity, specific heat, and thermal conductivity, respectively.  $\mathbf{f}$  is the external body force per unit mass, which can be defined as:  $\mathbf{f} = \mathbf{g}\beta(T - T_{ref})$

with the assumption of the Boussinesq approximation, where  $\mathbf{g}$  is the acceleration due to gravity,  $\beta$  is the volumetric thermal expansion coefficient, and  $T_{ref}$  is the reference temperature.

The latent heat source term  $q$  in the energy equation shown in Eq. (3) can be expressed as:

$$q = - \left[ \frac{\partial(\rho \Delta H)}{\partial t} + \nabla \cdot (\rho u \Delta H) \right] \quad (4)$$

in which  $H$  is the latent enthalpy of a computational cell undergoing phase change. Further, the liquid fraction is denoted by  $f_l$ , given as  $f_l = \Delta H/L$ , where  $L$  is the latent heat of melting. For a pure substance, the second term in Eq. (4) can be neglected and the latent heat source term becomes:

$$q = - \frac{\partial(\rho \Delta H)}{\partial t} = - \frac{\partial(\rho L f_l)}{\partial t} \quad (5)$$

## 2.2. Lattice Boltzmann BGK and MRT equations for density and velocity fields

In the LBM, separate particle distribution functions are used to compute the density (and velocity) and thermal fields. The distribution function is obtained by solving the lattice Boltzmann equation, which is a special discretization of the kinetic Boltzmann equation. The macroscopic quantities of the simulated fluid can be then derived by calculating the hydrodynamic moments of the distribution function. Unlike the second-order PDEs in the Navier-Stokes approach, the LBM uses only the first order PDEs, and the generalized lattice Boltzmann equation can be expressed as:

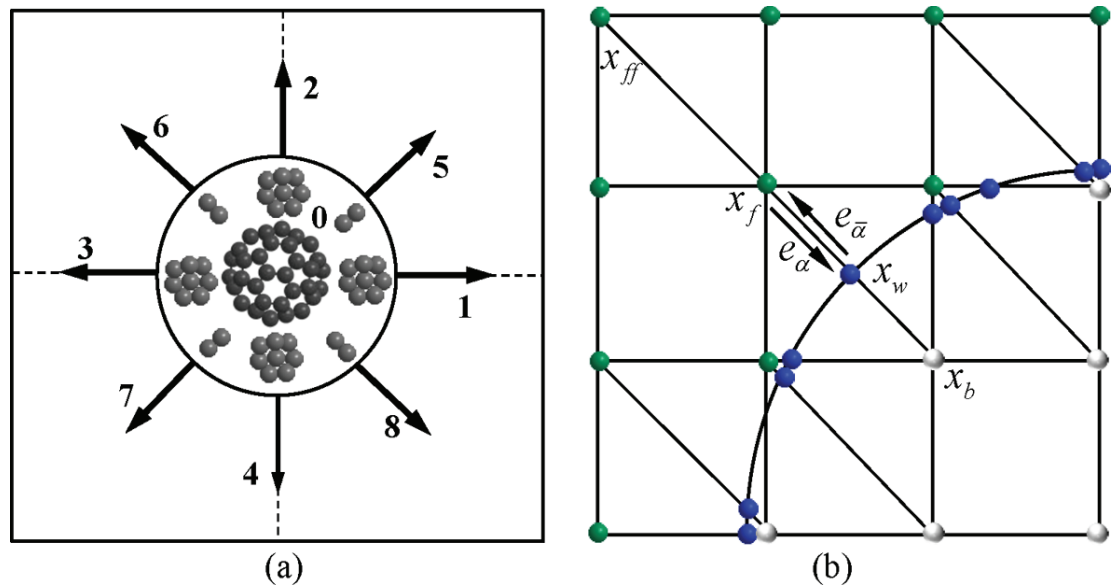
$$f(x + e\Delta t, t + \Delta t) - f(x, t) = \Delta t \times (\Omega + F) \quad (6)$$

where  $\mathbf{f}$  is the distribution function,  $\mathbf{e}$  is the microscopic velocity,  $\Omega$  is the collision operator, and  $\mathbf{F}$  is the external force.

In this work, the D2Q9 model is used for the discretization of velocity space for the two dimensional case. The nine velocities in the D2Q9 (Figure 1(a)) lattices are given by:

$$e_\alpha = \begin{cases} (0, 0) & \alpha=0 \\ c(\cos[(\alpha-1)\pi/2], \sin[(\alpha-1)\pi/2]) & \alpha=1,2,3,4 \\ \sqrt{2}c(\cos[(2\alpha-1)\pi/4], \sin[(2\alpha-1)\pi/4]) & \alpha=5,6,7,8 \end{cases} \quad (7)$$

in which  $\alpha$  is the streaming direction and  $c$  is the streaming speed, defined as  $c = \Delta x/\Delta t$ , where  $\Delta x$  and  $\Delta t$  are the lattice cell size and the lattice time step, respectively.



**Figure 1:** Spatial discretization (a) D2Q9 lattice used in a 2-D geometry and (b) curved boundary treatment.

For single relaxation time (BGK), the collision term in Eq. (6) will be replaced by the following expression:

$$\Omega = -[f(x, t) - f^{eq}(x, t)]/\tau_v \quad (8)$$

where  $f^{eq}$  is the equilibrium distribution function, and  $\tau_v$  is the relaxation time, computed from:

$$\tau_v = \frac{3\nu}{c^2\Delta t} + \frac{1}{2} \quad (9)$$

where  $\nu$  is the kinematic viscosity.

The equilibrium distribution function of Eq. (6) is expressed as:

$$f_\alpha^{eq} = \rho w_\alpha \left( 1 + \frac{3e_\alpha \cdot u}{c^2} + \frac{9(e_\alpha \cdot u)^2}{2c^4} - \frac{3u^2}{2c^2} \right) \quad (10)$$

where  $w_\alpha$  is the equilibrium distribution weight for direction  $\alpha$ , given as:

$$w_\alpha = \begin{cases} 4/9 & \alpha=0 \\ 1/9 & \alpha=1,2,3,4 \\ 1/36 & \alpha=5,6,7,8 \end{cases} \quad (11)$$

For MRT, the collision term in Eq. (6) can be expressed as:

$$\Omega = -\mathbf{M}^{-1} \mathbf{S}(\mathbf{m} - \mathbf{m}^{eq}) \quad (12)$$

where  $\mathbf{M}$  is the transformation matrix,  $\mathbf{S}$  is the diagonal matrix of non-negative relaxation rates, and  $\mathbf{m}$  and  $\mathbf{m}^{eq}$  represent the velocity moments of the distribution functions  $\mathbf{f}$  and their equilibria, respectively.

The basic quantities such as  $\mathbf{m}$ ,  $\mathbf{m}^{eq}$ ,  $\mathbf{M}$ , and  $\mathbf{S}$  are completely defined in [32], and we just provide the brief expressions of them. The physical signification of velocity moments in Eq. (12) is given as:

$$\mathbf{m} = (\rho, e, \epsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^T \quad (13)$$

and  $\mathbf{M}$  is a  $q \times q$  matrix, which linearly transforms the distribution functions  $\mathbf{f}$  to the velocity moments  $\mathbf{m}$ :

$$\mathbf{m} = \mathbf{M} \bullet \mathbf{f}, \quad \mathbf{f} = \mathbf{M}^{-1} \bullet \mathbf{m} \quad (14)$$

$\mathbf{S}$  is a non-negative  $q \times q$  diagonal relaxation matrix:

$$\mathbf{S} = \text{diag}(0, s_e, s_\epsilon, 0, s_q, 0, s_q, s_v, s_v) \quad (15)$$

In order to incorporate buoyancy force in the model, the Boussinesq approximation is applied. Therefore, the force term in Eq. (6) needs to be calculated as follows in the vertical direction ( $y$ ):

$$F_\alpha = 3w_\alpha g_y \beta T(x, t) \rho(x, t) e_{\alpha y} \quad (16)$$

Then, the fluid density  $\rho$  can be evaluated from Eq. (17a), whereas the velocity  $\mathbf{u}$  can be extracted from the momentum fluxes of Eq. (17b):

$$\rho = \sum_{\alpha} f_{\alpha} \quad (17a)$$

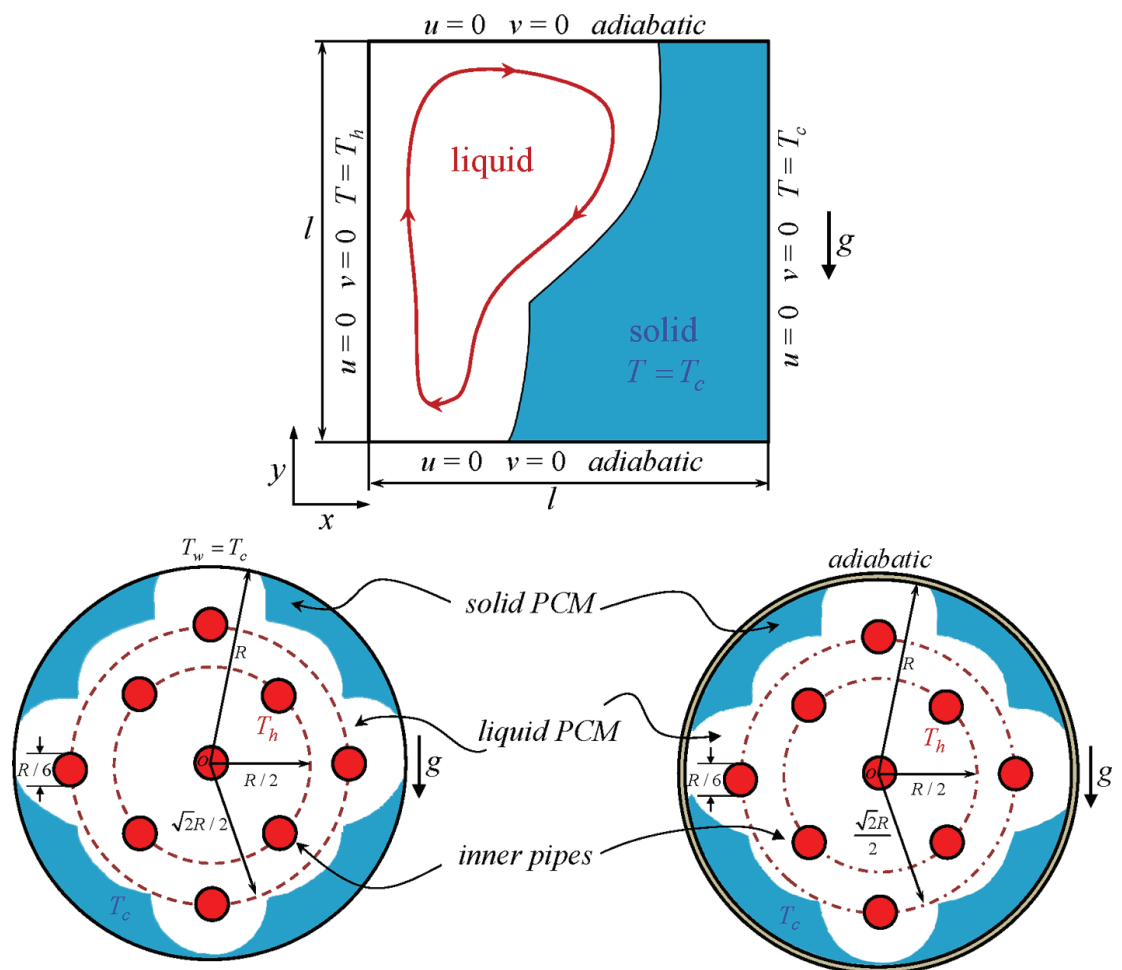
$$\rho u = \sum_{\alpha} e_{\alpha} f_{\alpha} \quad (17b)$$

In Figure 1(b), the curved boundary treatment illustration is provided. Detailed explanation of the non-equilibrium extrapolation scheme can be found in the work of Guo et al. [33].

Two computational domains are considered in this work: (1) a square cavity and (2) a shell and tube system. The first geometry is applied to validate the LBM code and test the performance of different LB models, and the second one is taken into account to extend the application of LBM to complex system and check the effects of the number and arrangement of inner tubes on multitube thermal energy storage systems.

As shown in Figure 2, the square cavity is initially uniformly filled with a solid chemical pure substance at the melting temperature  $T_c$ . The walls of the cavity are impermeable and no-slip. Horizontal walls are adiabatic, whereas the left and the right walls are set to the fixed temperatures, and  $T_h > T_c$ . The shell and tube system also uses the

pure substance with the inner tubes keeping at constant temperature of  $T_h$ , and the outer shell is at  $T_c$  or adiabatic as presented in Figure 2. Some assumptions are adopted to simplify this problem: (1) the fluid is incompressible, (2) densities of both phases are equal, (3) Boussinesq approximation is used, (4) liquid viscosity is constant, (5) specific heats of both solid and liquid phases are constant and equal, (6) both thermal conductivities are constant and equal, and (7) the solid phase is fixed to the walls.



**Figure 2:** Schematics of (top) cavity and (bottom) shell and tube model with constant temperature and adiabatic boundary conditions.

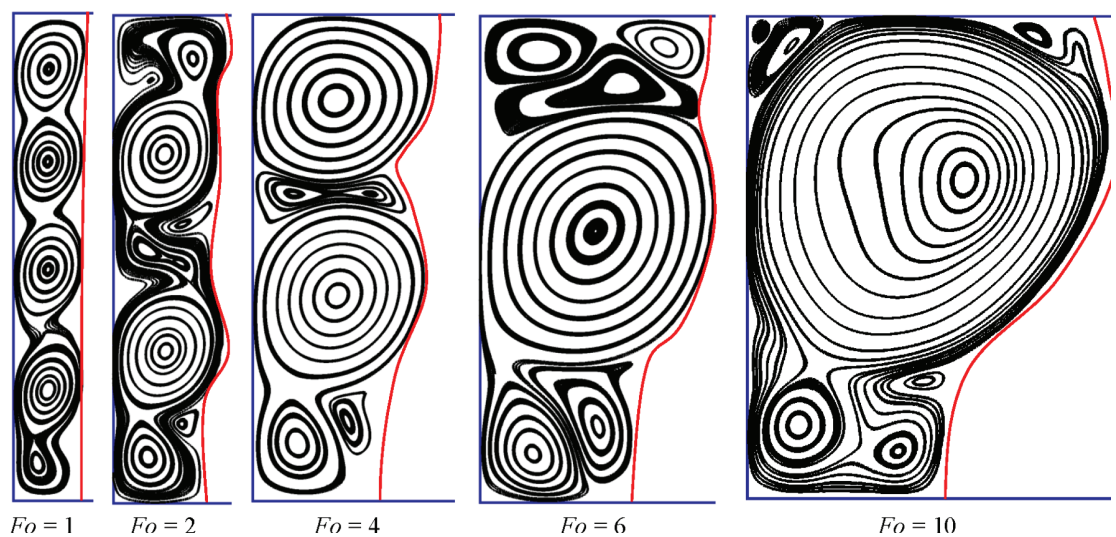
### 3. Results

#### 3.1. Convection melting in cavity model

The numerical simulations of melting with convection are performed in a square cavity, that have been done by many scholars [18, 26, 29]. Some basic information and



assumptions about the cavity model are given. In this problem, two instability mechanisms must be considered. One mechanism is the nonphysical oscillation, which can be attributed to numerical scheme. Another one is the high frequency oscillation, which may be caused by the evolution of the circulation cells as melting proceeds. In detail, the multi-cellular (multi-vortices) flow is unsteady with small vortices generating and vanishing as melting proceeds (Figure 3). We first verify the accuracy and stability of LB code by comparison with benchmark results presented in [18]. Then, the numerical performances of different LBMs for phase change problem are tested.

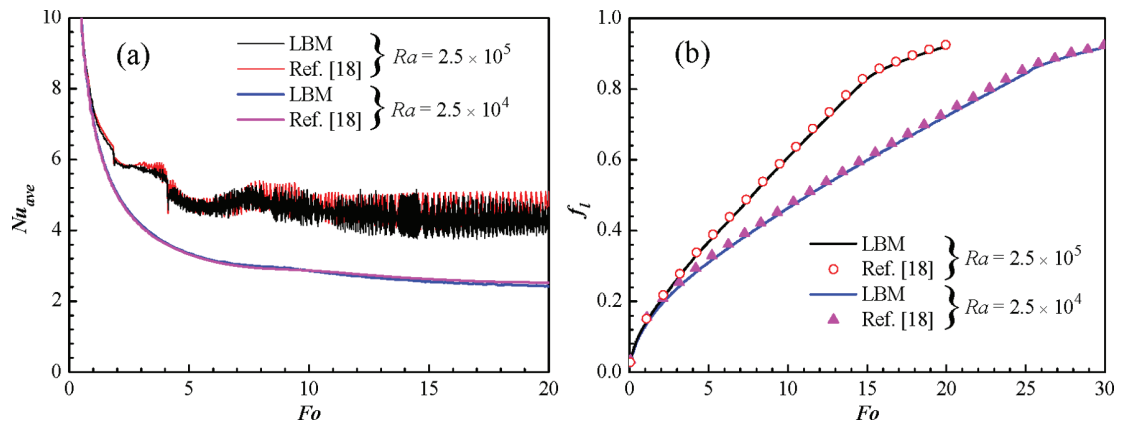


**Figure 3:** Convection melting in cavity: Interfaces and streamlines by LBM at different non-dimensional times  $Fo$  (from left to right: 1, 2, 4, 6, and 10) at  $Pr = 0.02$ ,  $St = 0.01$ , and  $Ra = 2.5 \times 10^5$ .

Figure 4 gives the comparison of LBM results with Mencinger's results by adaptive grid method [18] for the case:  $Pr = 0.02$ ,  $St = 0.01$ ,  $Ra = 2.5 \times 10^4$  and  $2.5 \times 10^5$ , and a good agreement of the evolution of average Nusselt number ( $Nu_{ave}$ ) and total liquid fraction ( $fl$ ) can be observed. As shown in Figure 4(a), the  $Nu_{ave}$  tends to decrease over time due to the competition between pure conduction and natural convection, and it suffers from high frequency oscillation with the increase of the Fourier number ( $Fo$ ) at  $Ra = 2.5 \times 10^5$ , which has been reported by many other researchers [26]. Besides, the total liquid fraction is less sensitive and more stable than the Nusselt number as presented in Figure 4(b), and agrees well with Mencinger's results [18] with maximum relative difference less than 1%. These results demonstrate that the LBM we adopt in this work is suitable for solid-liquid phase change problems.

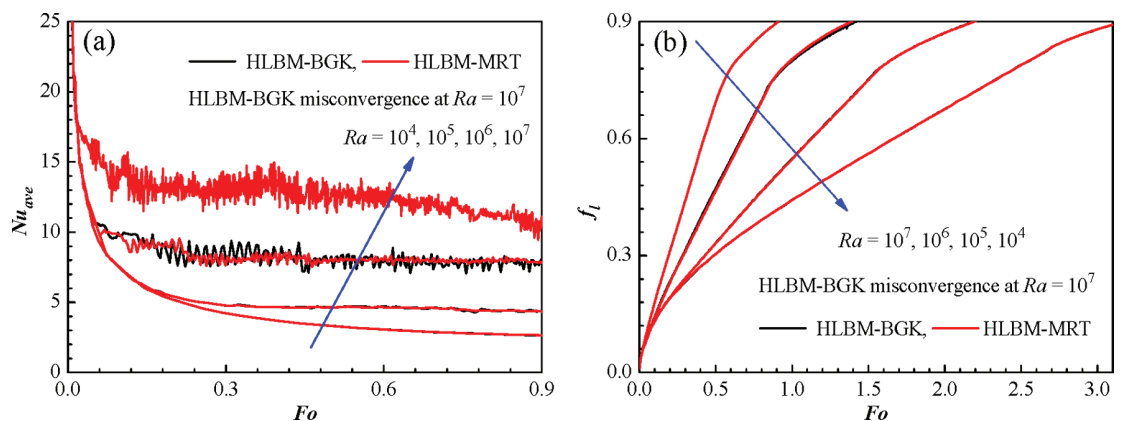
The numerical performance of BGK and MRT models is tested for the case of phase change with natural convection, varying  $Ra$  from  $10^4$  to  $10^7$  for  $Pr = 0.1$  and  $St = 0.1$ . Figure 5 shows the results of the average Nusselt number and total liquid fraction. At a low value of  $Ra = 10^4$ , the convective heat transfer is obviously inhibited, and





**Figure 4:** Validation of LBM code: (a) the average Nusselt numbers along the left wall, and (b) total liquid fraction for  $Pr = 0.02$ ,  $St = 0.01$ ,  $Ra = 2.5 \times 10^4$ , and  $Ra = 2.5 \times 10^5$ .

both the BGK and MRT models can obtain stable results as shown in Figure 5(a). With the increase of  $Ra$ , the flow of liquid phase is enhanced and the BGK results become unstable under the combined effects of nonphysical oscillation and high frequency oscillation, and finally, the BGK solution for  $Ra = 10^7$  becomes divergent. But the MRT model can obtain convergent numerical results in a wider range of  $Ra$ . It can be seen from Figure 5(b) that the difference of total liquid fraction between the BGK and MRT is small, which means that the accuracy of these two LB models is close, but the MRT is much more stable than BGK, especially for the case of high  $Ra$  number.



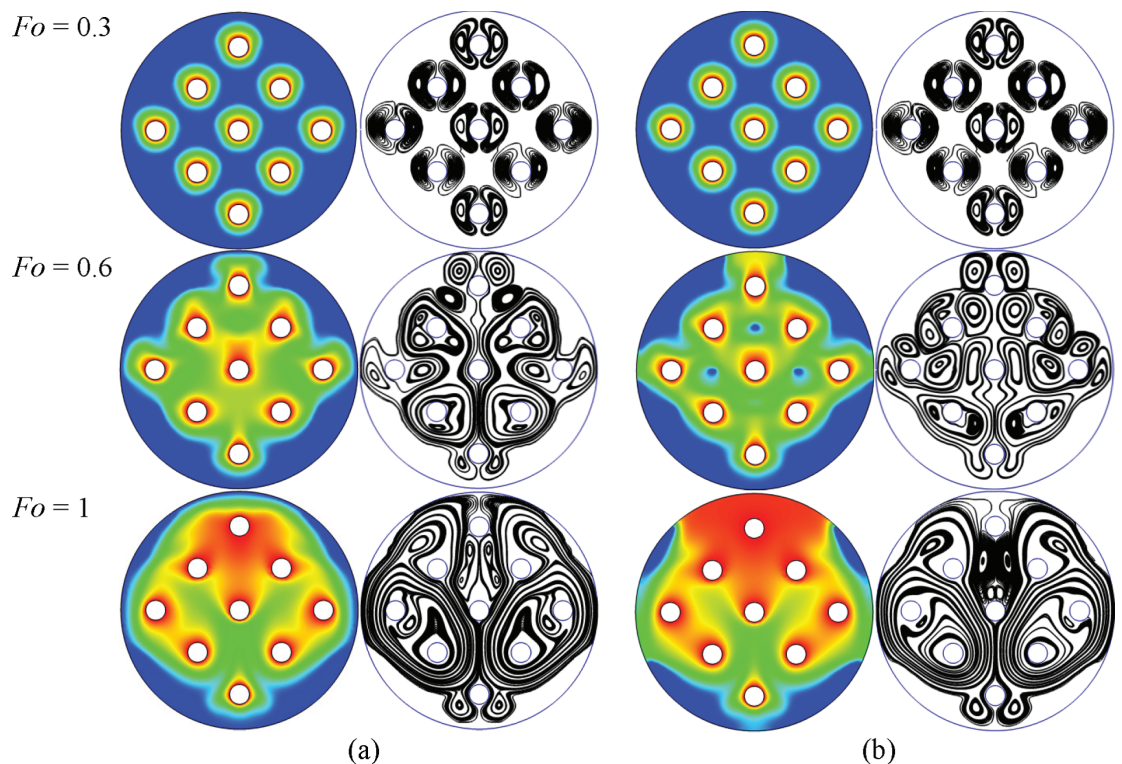
**Figure 5:** Comparison of lattice Boltzmann BGK and MRT models: (a) average Nusselt numbers along the left wall, and (b) total liquid fraction for  $Pr = 0.1$ ,  $St = 0.1$  at different  $Ra$  numbers.

### 3.2. Convection melting in shell and tube heat storage system

Most of lattice Boltzmann simulations for the phase change problems have been done in a cavity, and few studies concern more complex geometries. In fact, Agyenim et al. [7], in a critical review of PCM containers, pointed out that the PCMs are typically placed

in four types of containers: long thin heat pipes, cylindrical containers, rectangular containers, and spherical containers. Among them, the shell and tube system is most intensely used in latent heat thermal energy storage system, accounting for more than 70%, if the source of energy is a solar collector. Therefore, we extend the application of the LBM to complex shell and tube heat storage system, and test the heat transfer performance of various numbers and arrangements of the tubes.

Figure 6 illustrates the dimensionless temperature and streamlines at different  $Fo$  with Dirichlet and adiabatic boundary conditions of the shell. Results have been obtained for  $Pr = 0.1$ ,  $St = 0.01$ , and  $Ra = 10^5$ . As shown in Figure 6, the overall melting process in the multitube system can be broken down into three stages. At the first stage, convection is inhibited and heat transfer remains essentially that of conduction, and several couples of crescent-shaped can be observed in the flow field. With the increase of liquid phase fraction, the convective heat transfer is enhanced, and the streamlines appear as a mask consisting of different sizes of vortexes. Then, convection becomes dominated, characterized by liquid region above the heat transfer tube and a solid region below, and finally, convection dominated zone fills the entire volume of the multitube system.



**Figure 6:** Dimensionless temperature and streamlines at different  $Fo$  with (a) constant temperature boundary condition and (b) adiabatic boundary condition for  $Pr = 0.1$ ,  $St = 0.01$ , and  $Ra = 10^5$ .

## 4. Conclusion

Phase change phenomenon in a single-component system has been computationally handled in a generalized lattice Boltzmann framework. By testing and analyzing different LB models, we have found that the dual distributions HLBM-MRT scheme is more suitable for convection dominated melting process. In the scheme, the enthalpy-based lattice Boltzmann model with basic evolution variable of enthalpy (HLBM) for thermal field avoids the sink (melting) term in the collision step, and the multiple relaxation time (MRT) model for flow field overcomes numerical instability and inaccurate boundary. Results obtained from the present study are highly consistent with the numerical results obtained by an adaptive grid method in the literature.

Lattice Boltzmann simulation for the phase change problems has been extended to more complex geometries, that is, a shell and tube latent heat storage system, and the heat transfer performance has been tested. Numerical results show that the heat transfer is greatly enhanced in a multitube system compared to that of the single tube due to the larger heat transfer surface area.

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